Inside out *Porphyridium cruentum*: beyond the conventional biorefinery concept

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Table S1. Data collection and refinement statistics.

Data collection	
Space group	R3
a=b, c (Å)	186.590, 59.190
α=β, γ (°)	90.0, 120.0
Molecules for asymmetric unit	Two αβ dimers
Observed reflections	925709 (44973)
Unique reflections	100909 (5012)
Resolution (Å)	46.65– 1.60 (1.62– 1.60)
Completeness (%)	99.0 (98.3)
Rmerge (%)	0.101 (1.028)
Average I/σ(I)	12.9 (2.2)
Multiplicity	9.2 (9.0)
$CC_{1\backslash 2}$	0.997 (0.595)
Refinement	
Resolution (Å)	46.65 -1.60
N° reflections	95441
N° reflections in working set	6986
Rfactor/Rfree	0.223/0.256
N° non-H atoms in the refinement	5990
B-factor overall ($Å^2$)	18.1
Average B-factor	23.93
Ramachandran values (%)	
Most favoured/ Additional allowed	97.19
Outliers	0.62
R.m.s.d. from ideality	
R.m.s.d. bonds (Å)	0.010
R.m.s.d. angles (°)	1.602

Figure S1. PE crystals. Crystals were grown by hanging drop vapor diffusion method using a drop containing 10 mg/mL PE in 0.250 M ammonium sulphate, 0.025 M potassium phosphate at pH 5.0, equilibrated with a reservoir containing 0.500 M ammonium sulphate, 0.050 M potassium phosphate at pH 5.0.

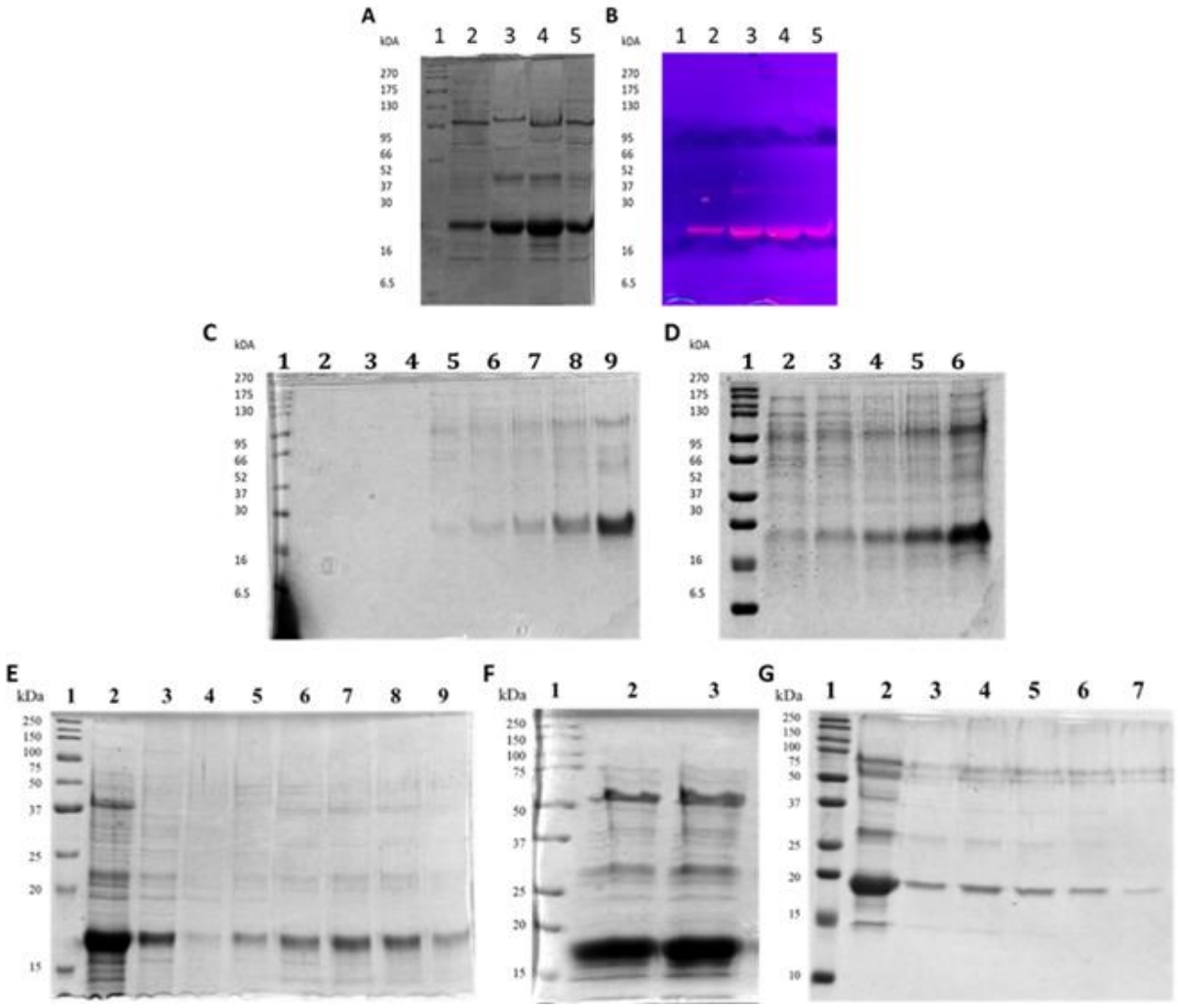

Figure S2. PE extraction and purification. Coomassie stained (**A**) and UVA light exposed unstained (**B**) SDS-PAGE analysis of total proteins extracted with different techniques. Lane 1: protein molecular weight markers; lane 2: Freeze & thaw extract; lane 3: Ultrasound extract; lane 4: Maceration extract; lane 5: French Press extract. 30 µg of total proteins were loaded in each lane. **C, D,** Coomassie staining of SDS-PAGE. Proteins were extracted by ultrasounds for different times. **(C)** fresh biomass and **(D)** frozen biomass. **C:** Lane 1: protein molecular weight markers; lanes 2-4: empty lanes; lanes 5-9: proteins extracted for 4, 8, 12, 16, and 20 minutes, respectively. **D:** Lane 1: protein molecular weight markers; lanes 2-6: proteins extracted for 4, 8, 12, 16, and 20 minutes, respectively. **E-G.** SDS-PAGE analysis of different procedures to isolate PE from *P. cruentum*. **E**: Anion-exchange. Lane 1: molecular weight markers; lane 2: total protein extract, lane 3: unbound; lane 4: washing fraction 1; lane 5: washing fraction 3; lane 6-9: samples eluted by 0.25 M NaCl. **F**: Ultrafiltration. Lane 1: molecular weight markers; lane 2: total protein extract; lane 3: ultrafiltration retentate. **G**: Size exclusion chromatography. Lane 1: molecular weight markers; lane 2: total protein extract; lanes 3-7: samples eluted from gel filtration. In all lanes, 30 µg of total proteins were analyzed.

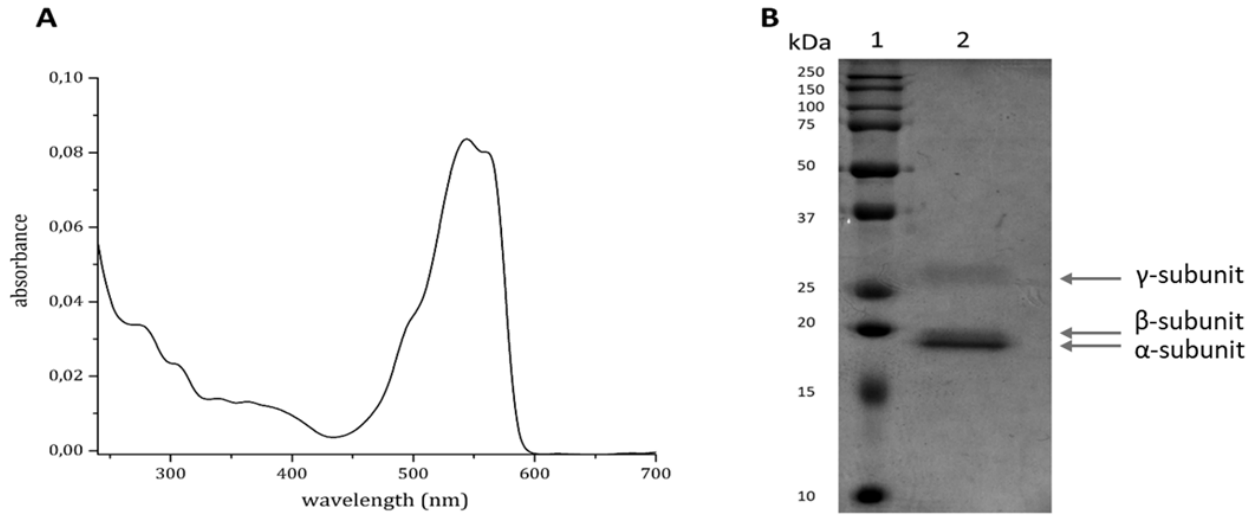

Figure S3. Analyses of PE dissolved crystals. A: UV-vis spectrum obtained from PE dissolved crystals. Spectrum was acquired at 25 °C, in the range 400–700 nm. **B**: SDS-PAGE analyses of PE dissolved crystals. Lane 1: molecular weight markers; lane 2: 20 μL of PE dissolved crystals.

Table S2. Tentatively identified compounds from *P. cruentum* extracts by HPLC-DAD-APCI-QTOF-MS/MS analysis, including peak annotation, high-resolution mass spectrometry features and UV–Vis maxima.

Peak	RT (min)	Identification	Experimental $[M + H]^+$ *m/z*	UV–Vis maxima (nm)	MS/MS product ions
1	3.471	Chlorophyll derivative I	549.4875	340s, 380s, 428	307.1400, 97.1048
2	4.177	Chlorophyll derivative II	549.4871	340s, 380s, 428	305.1354, 255.0720
3	6.658	Phaeophorbid B, methyl ester	623.2851	420	565.2795, 499.2056
4	7.347	Pheophytin derivative	909.5374	340s, 380s, 428	631.2374, 559.2071
5	7.668	Zeaxanthin isomer I	569.4357	422, 446, 474	464.8067, 281.2215, 175.1480
6	8.057	Zeaxanthin	569.4342	420s, 445, 476	423.3309, 338.2549, 175.1480
7	9.826	Zeaxanthin isomer II	569.4365	422, 446, 474	539.4249, 175.1480
8	11.920	3-Acetylpheophytin a	887.5709	410	609.2687, 549.2495
9	13.621	Divinyl pheophytin a	869.5547	410	592.2652, 487.1950
10	14.656	Plastoquinone	749.6235	420	551.3212, 495.2654, 151.0743
11	14.862	Pheophytin b	885.5527	420	607.2536, 503.2403
12	16.500	Pheophytin a	871.5739	420	594.2828, 533.2567
13	18.701	β-Carotene	537.4441	420s, 450, 480	375.2935, 173.1293
14	18.892	β-Carotene isomer	537.4456	420s, 450, 480	261.1637, 146.1004